

N-Butylnitrite
544-16-1 | DTXSID8049418

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 1.46

Global applicability domain: Inside

Local applicability domain index: 6.15e-01

Confidence level: 8.14e-01

Nearest Neighbors from the Training Set

Image not found

1-Nitrobutane

Measured: 1.47

Predicted: 1.35

Image not found

Propane, 2-methyl-1-nitro-

Measured: 1.40

Predicted: 1.42

Image not found

1-Nitropentane

Measured: 2.01

Predicted: 1.83

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Propane, 2-methyl-2-nitro-

Measured: 1.17

Predicted: 1.33

Image not found

2-Nitrobutane

Measured: 1.20

Predicted: 1.33